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A Modernized Version of a 1D Soil Vegetation Atmosphere Transfer model for improving its future use in Land Surface Interactions Studies

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ABSTRACT

SimSphere is a land biosphere model that provides a mathematical representation of vertical 'views' of the physical mechanisms controlling Earth's energy and mass transfers in the soil/vegetation/atmosphere continuum. Herein, we present recent advancements introduced to SimSphere code, aiming at making its use more integrated to the automation of processes within High Performance Computing (HPC) that allows using the model at large scale. In particular, a new interface to the model is presented, so-called "SimSphere-SOA" which forms a command line land biosphere tool, a Web Service interface and a parameters verification facade that offers a standardised environment for specification execution and result retrieval of a typical model simulation based on Service Oriented Architecture (SOA). SimSphere-SOA library can now execute various simulations in parallel. This allows exploitation of the tool in a simple and efficient way in comparison to the currently distributed approach. In SimSphere-SOA, an Application Programming Interface (API) is also provided to execute simulations that can be publicly consumed. Finally this API is exported as a Web Service for remotely executing simulations through web based tools. This way a simulation by the model can be executed efficiently and subsequently the model simulation outputs may be used in any kind of relevant analysis required.

The use of these new functionalities offered by SimSphere-SOA is also demonstrated using a "real world" simulation configuration file. The inclusion of those new functions in SimSphere are of considerable importance in the light of the model's expanding use worldwide as an educational and research tool.

Keywords: *SimSphere, SVAT, land surface interactions, Service Oriented Architecture, Web Service, software developments, Earth Observation*

1. Introduction

Land surface interactions govern the critical exchanges of energy and mass between the terrestrial biosphere and the atmosphere, and are major drivers of the Earth's system (Jung et al., 2011; North et al., 2015). There is an urgent need today for a better understanding and a more accurate monitoring of Earth's natural processes and interactions, evidently strengthened even more in the face of pressures from climate change and global food and water security (Coudert et al., 2008; Ireland et al., 2015; Mannschatz et al., 2016). The growing role of simulation in Earth systems science together with the increasing available computing power have resulted to an increase in the complexity of processes included in the design of simulators (Coon et al., 2016).

Land Surface Parameterisation schemes (LSPs, also known as Land Surface Models, LSMs) are one of the preferred scientific tools to quantify earth system interactions at different spatial and temporal resolutions. LSPs simulate a number of parameters characterising land surface interactions within the lower atmospheric boundary from a predefined set of surface characteristics (i.e. properties of soil, vegetation and water). One such group of LSPs includes Soil-Vegetation-Atmosphere Transfer (SVAT) models. Those mathematical models provide representation of vertical 'views' of the physical mechanisms controlling energy and mass transfers in the soil-vegetation-atmosphere continuum. SVATs provide estimates of the time course of soil and vegetation state variables at time-steps compatible with the dynamics of atmospheric processes. Also are able to describe the multifarious transfer processes through varying degrees of complexity, over different temporal and spatial scales (Ridler et al., 2012).

SimSphere is an example of a 1-D SVAT model, originally developed by Carlson and Boland (1978) and Lynn and Carlson (1990), and considerably modified to its current state with its latest version written in Java by Gillies et al., (1997) and Petropoulos et al., (2013a). Since its development it has been utilised in studies concerning the study of land surface interactions (North et al., 2015) and the examination of hypothetical scenarios studying feedback processes (Grantz et al., 1999). Furthermore, it has been used synergistically with Earth Observation (EO) data to derive spatiotemporal estimates of energy fluxes and/or soil moisture (Carlson, 2007). Variants of this technique are currently investigated by Space Agencies for developing related operational products (Chauhan et al., 2003; Piles et al., 2011; ESA STSE, 2012; Piles et al., 2016). An overview of the model use can be found in Petropoulos et al., (2009a).

Behind SimSphere's Graphical User Interface (GUI) lies an engine that executes the computation of a number of output parameters after a set of input parameters are provided by the user from the User Interface (UI). The computation engine is a direct port from an existing Fortran 77 codebase to Java 1.3. This port was originally undertaken 15 years ago, and during that time the code base has been amended with various computation routines by various developers for a number of applicational purposes. Moreover the GUI code is entangled with the logic of the computation engine and provides a custom interface by providing a set of parameters as an input to the computation routines. The introduction of Service Oriented Architecture (SOA) practices in the remote sensing realm is relatively new (El-Sharkawi et al., 2013). Modern execution environments, like cloud platforms or numerical computation Domain Specific Languages (DSLs), like Modelica, are not able to create value from the research work in the codebase mostly due to a monolithic, standards in compliant approach. One can attribute the problem to the lack of SOA design. This is also related to the porting of business logic from old programming languages, like Fortran 77, which contributes much syntactic noise. SOA allows the service specification and modularity in a multi-lingual environment. The SOA rules outlined in Bell (2008) and Schroth and Janner, (2007) could potentially serve to improve the separation of roles. According to these authors, the researcher is not a developer and vice versa. Both roles have their own domain

specific knowledge and skills and through SOA the developer can create a standardised interface that exposes the business logic engineered by the researcher. This can be done through protocols and standards, something that SOA reinforces.

In the purview of the above, the aim of this work has been to apply modern trends in software development to an existing codebase in the field of EO and land surface modeling to outline an SOA migration path, display its benefits and improve the software quality. SimSphere is an ideal example to be chosen as a case study as it is widely adopted in research, its use is rapidly expanding worldwide, and, the software toolkit is minimal enough to have a proof-of-concept, while rich enough to display our approach. More specifically, the existing GUI code is removed from the model and then SOA design patterns are applied in order to create a command line implementation suitable for cloud deployments or High Performance Computing (HPC) execution, which subsequently exposes the model functionality as a service.

2. SimSphere Description

SimSphere is a one-dimensional land biosphere model. It simulates a series of physical processes that take place as a function of time in a column that extends from the soil root zone up to a level higher than the surface vegetation canopy. Three main systems within the models' architecture, include the *physical*, the *vertical* and the *horizontal* layers (**Figure 1**). The *physical* components ultimately determines the microclimate conditions in the model, grouped into three categories, *radiative*, *atmospheric* and *hydrological*. The *vertical structure* components, effectively correspond to the Planetary Boundary Layer (PBL) and are divided into three layers - a surface mixing layer, a surface of constant flux layer and a surface vegetation or bare soil layer, where the depths of the first layer is somewhat variable with time, growing throughout the day as sensible heat is added from below. The depth of the constant flux and vegetation layers are set in the model input, although the depth of a bare soil transition (between soil and air) layer is variable in time depending on the wind speed and the surface roughness. The substrate layer refers to the depth of the soil over which heat and water is conducted. The processes and interactions simulated by SimSphere develop over a 24-h diurnal cycle at a chosen time step, starting from a set of initial conditions given in the early morning (at 05.30 am local time) with a continuous evolving interaction between soil, plant and atmosphere layers. A number of input parameters are required to parameterise the model, categorised into 7 defined groups (**Table 1**). Model provides predictions as a function of time for a total of more than 30 variables (**Table 2**). A detailed description of SimSphere architecture can be found in Gillies (1993). The current version of the model is globally distributed from Aberystwyth University, UK (<http://www.aber.ac.uk/simsphere>).

3. Existing Structure and Architecture of SimSphere

The development of SimSphere-SOA has primarily been motivated by efforts to increase the usability of the original software model. In its currently distributed version of SimSphere, the GUI code was written as a presentation and configuration layer to an Extensible Markup Language file. This XML file provided the configuration layer of the data, whilst the persistency layer that transformed user data to the XML file and back was written by hand using custom data types. A component to a server based proprietary execution environment was also developed, but SimSphere software is typically used as a desktop application. The interface to the Fortran 77 computational logic was done through a function which took all the arguments used for the computation as inputs. In **Figure 2** is provided an overview of the current architecture. From it

and the usage of the software, it can be observed that there is room for further improvements in the original SimSphere software toolkit and in particular:

- There is no way for exporting the model inversion data.
- The configuration (that configures the internal data-structures with user input) and validation layer (that examines user input for errors) is manually written which is error prone.
- The UI couples tightly with the validation and persistency layer (that loads specification and save results) . No third party interface for other UIs is possible.
- There are two parts in the validation layer. The first is manually written and the other is written on old technology (Document Type Definition, DTD).
- The application is not available for headless installations because of the UI coupling.
- The application cannot be used remotely through Web Services.
- Uses legacy unsupported code.
- The application cannot be run in HPC or in batch mode.

There are also a number of other possible issues to address on the model distributed version not evident in **Figure 2** that mainly pertain to maintainability. Typically current deprecated methods do not work as expected and make functionalities of the software unusable in current versions of Java. It is also obvious from the code base that an entangling of roles leads to major shortcomings in the development process.

4. SimSphere-SOA Developments

The newly developed code within SimSphere-SOA was structured to follow the SOA principles. For the computational logic layer an orchestrator was created, behind a mega-function interface, which uses the services of the persistency layer to read the XML and export the results of the computation to a Comma Separated Values (CSV) formatted file (Shafranovich, 2005). The new model architecture is shown in **Figure 3**. As an SOA approach, SimSphere-SOA provides the service of simulation by consuming messages in XML format and producing messages in CSV format, allowing them to be consumed by a third party application. Using the self-documenting configuration and validation layer, various applications can be designed around the Application Programming Interface (API) as illustrated in **Figure 4**.

There are two endpoints per CSV. The first one takes the XML file as input and produces a CSV of a time based simulation for a whole day. The first column is the simulation time in 15-minute (or higher) steps, whereas the remaining columns contain the evolution of various geophysical quantities as samples at these time instances. The second type of simulation runs various scenarios for a specific time of a particular day encoded as Fractional Vegetation Cover (FVC) and Surface Moisture Availability pairs. These two quantities vary in the 0.1 floating point range. The user can specify steps to sweep the two ranges independently, and for each combination of values, quantities of interest to the remote sensing community are computed. The results are exported as a CSV in the desktop version; however the application can run also as a server where it exposes the two endpoints as shown in **Table 3**. The request headers should be Content Type: application/xml and Accept: text/csv. This last step can be used for fast model inversion.

Apart from the various Computer Science (CS) considerations, this new application is an enabler for sophisticated Sensitivity Analysis (SA) tooling in SimSphere. This is very important functionality in terms of future efforts related to performing an all-inclusive the verification of the model. Indeed, SA can help to understand the behavior of a model and in establishing the dependency of the model outputs on its input parameters in how different parts of the model interplay. By means of an SA, irrelevant parts of the model may be dropped or a simpler model can be built or extracted from a more complex one (so-called model lumping), reducing, in some cases significantly, the required computing power in running a model. SA also provides a valuable method to identify critical input parameters and rank them in order of importance. The latter can offer important guidance to the design of experimental programs as well as to more efficient model coding or calibration (e.g. Petropoulos et al. 2009b; 2013b). The new model architecture presented herein allows the creation of a generalised SA scheme which decouples the application from executing various runs manually in order to derive the results. As SimSphere is provided as a service, one needs to change the XML files, create CSV files and run the analysis algorithm via a scripting mechanism. SimSphere-SOA is completely stateless (two executions of SimSphere are independent) and is suitable for HPC environments, since it creates a stateless cluster (as illustrated in **Figure 5**).

5. SimSphere-SOA Software Availability

SimSphere-SOA product has been also developed as open source software, as its predecessor SimSphere, and is hence, released under the terms of the GNU General Public License. The software code of this new model version is also freely distributed from the main web site from where the model is distributed globally maintained by Aberystwyth University, UK (www.aber.ac.uk/simsphere).

6. Implementation

6.1. Validation layer

A smaller software tool was created to amend and improve upon SimSphere original model architecture, whilst also ensuring that SOA guidelines and use standards were respected in order to facilitate and the work of the EO community. As a first step, the two validation layers that existed in the currently distributed model version were unified into a single layer in SimSphere-SOA. The two validation layers were very different; one was contained within the application while the other one was external. In order to extract the internal validation layer, amendments to the original code had to be made. Following assessment of the code, the requirements for the unified validation layer which were not met by the existing approach were identified as the following:

- The data types of the XML should be specified.
- The validation layer should be self-documenting for a developer.
- The validation layer should include comments for the non-developer end users.
- The validation layer must lie externally to application in order to meet the previous requirements.

- The validation layer should be used by the software before using the data for computations.
- The validation should be standardised.

Having identified these requirements, the XML Schema Definition (XSD) version 1.1 was utilised for the application. Compared to the previous version 1.0, the updated version has the added value of the inclusion of validation, which was previously available as the separate Schematron standard. Using this solution, the validation logic could be externalised as a self-documenting, easily comprehensible compact document. The other benefit is that the same document could be used to create a persistent layer. In the case of SimSphere-SOA, the XSD file contained 3 more validation rules because extra domain specific knowledge from the expert, which is not encoded in the code base, was included. The new validation/persistency approach could also find validation errors that were not possible in the previous approach and were identified as bugs leading to runtime crashes, or worse, incorrect results. Both the newly developed and the existing approach was largely based on data types and their constraints. Perhaps the strongest advantage over the existing SimSphere application is the Look Up Table (LUT) functionality with selection among discrete alternatives and uniqueness provided by XSD 1.0 specification and does not exist in DTD specification. The XSD 1.1 specification facilitated the assertions outlined in **Table 4** which was not available in the previous version. There were also gains in readability. The Longitude element is a typical example. In our case, this is compactly represented as an XSD data type with upper and lower bounds (**Table 5**). In the old approach, this information was encoded in an XML file which resulted in the rule being copied between XML files with the risk of possible typographic mistakes. In the new approach, the XML corresponding element is simplified as one can see from **Table 6**, with evident gains in readability and robustness. The documentation of various XML parameters through the excellent xs3p package allowed for the web presentation to be easily highlighted and formatted.

6.2. Serialisation layer

While the Java Architecture for XML Binding (JAXB) API does not support version 1.1 of the XSD (XML Schema) specification, the assertions present in 1.1 could be commented out to create the 1.0 conforming document. In this respect, the serialisation layer was automatically generated as a Java package from the 1.0 document. Programmatically, given a conforming XML, the relevant classes specified through the 1.1 XSD version could be filled with the XML data. The corresponding classes in the old version were analysed by the cloc tool (CLOC). The results are shown in **Table 7**.

It should be noted that in the XSD, despite the validation and serialisation specification being roughly four times bigger in terms of lines of code in comparison to the DTD approach, as opposed to the manually generated Java it is almost four times smaller in terms of lines of code, and does not require Java expertise. Moreover the validation logic is contained within a single file in contrast to the previous approach which amounted to 39 different files (including DTD). Even if the logic in the XSD were more modularised, spanning multiple files for readability, the overhead would be minimal. The new configuration and validation layer is self-documenting and the validation could be done with the third party library Apache Xerces (Apache Xerces). Notably, application specific validation was not relied upon. There were also significant improvements related to the XML files in comparison to the original approach. The sample XML which was provided with the application had been reduced by 3.5 times in terms of file size in comparison to the original (**Table 7**).

With regards to the presentation layer, due to deprecated features and bugs, the GUI code had to be re-written. Instead of using this costly approach in the short term, a standards compliance was adopted to tackle the problem. It was observed that the outputs were double valued, in column form. Given that the model could simulate the 24 hours of a day at 15 minutes resolution, a uniform column based tabulation was available. The most widely used form for such data is the CSV format, which is a standard format supported by dozens of software. Consequently a solution was engineered to convert the internal representation in CSV format for output. The export functionality was not present in the previous approach. Through CSV, the presentation was delegated to other well-established and maintained tools such as LibreOffice.

6.3. Demonstration of new functions

In order to demonstrate the new functions offered by SimSphere-SOA a simulation configuration file was used for the case of running a simulation for Borgo Cioffi Italian experimental site (latitude 40.617 and longitude 14.933) specifically for the date 17 November 2004. After the conversion it could be used the xsd to identify various mistakes (**Figure 6**) that went uncaught by the standard SimSphere distribution. After correcting these mistakes the next challenge was related to the sounding atmospheric profile data provision. In the standard SimSphere distribution, the user has to manually provide such sounding data. They are typically taken from the Department of Atmospheric Science of the University of Wyoming. These come in a standard format. Here in the soundings were acquired for the corresponding date from the nearby weather station, namely LIRE. The provided data were saved to a .csv file and using an accompanying utility in the SimSphere-SOA distribution, namely csv2soundingset.java, it automatically generated the <SoundingSet> element in the correct format and units suitable for SimSphere-SOA (**Figure 7**). This was not possible in the standard version, as the user must employ a manual, error prone procedure. The tool respects the constraint posed by the core of Simsphere which is a limit of 51 Sounding elements. Also, notably the previous version had only 11 manually converted measurements. After checking the .xml file again for correctness via the XSD file, it was used to perform simulations. A .csv file was effortlessly generated that encoded the results of the simulation. A standard spreadsheet program was used to create the figures, namely MS Excel. The .xml used to generate the simulation results, namely sample.xml, is available at the corresponding Github project in the folder simsphere_xsd. An example prediction of the time evolution of Sensible Heat Flux of this day is illustrated in **Figure 8**.

7. Conclusions & Future Work

Herein, the applicability of the SOA architecture to a SVAT modeling tool was demonstrated. The innovation of the approach described herein is the exporting of validation logic encoded in code to an XSD. XSD can capture these constraints while the previous DTD validation could not. With XSD more accurate sensitivity analysis and model outputs validation can be performed while the user can use the inline documentation in order to insert valid values. Even if the input is erroneous, by using standard validation interfaces of XML editors the user can accurately describe and comfortably validate the input before submitting it. The validation could be used as a portable interface generator between developers. In the previous SimSphere product edition, manually generated Java code had to be exchanged. In contrast, the new SimSphere-SOA allows the user to analyse the input from the .csv provided as output which are compatible with numerous applications. The executions can be run in headless environments (for example in HPC) in parallel or through shell scripts.

SimSphere-SOA development has also resulted in the improvement in the maintainability of the application, code reduction and flexibility of the original model. The improvement in maintainability and code size is due to the automated validation and generation of a persistency

layer, whereas the flexibility owes its improvement to the SOA design. Moreover, the stateless nature of SimSphere-SOA allows it to scale in HPC environments. The stateless is expressed by the creation of two .csv files per XML which can be executed in parallel. While the first .csv allows the observation of time evolution, the second one is very important in running model inversion.

Future work may focus on the GUI re-design using modern practices and technologies that have proved their values. For this purpose a number of options can be explored including Java FX technology (current on-going implementation) or the more standardised approach of HTML5/EcmaScript6 following the web centric trend. A perhaps more pressing issue with SimSphere is related to the maintainability of the scientific investment in computational logic. In order to successfully separate the role of developer and researcher, future work on the model will be required to transform the code base to a researcher friendly DSL like OpenModelica. This development will be of key value in demonstrating a workflow that brings together the developer and the researcher with minimum overlap of responsibilities to each other.

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References

- Bell, M. (2008). Introduction to Service-Oriented Modeling. Service-Oriented Modeling: Service Analysis, Design, and Architecture. Wiley & Sons. p. 3. ISBN 978-0-470-14111-3.
- Carlson, T. (2007). An overview of the "triangle method" for estimating surface evapotranspiration and soil moisture from satellite imagery. *Sensors*, 7(8), 1612-1629.
- Carlson, T. N., & Boland, F. E. (1978). Analysis of urban-rural canopy using a surface heat flux/temperature model. *Journal of Applied Meteorology*, 17(7), 998-1013.
- Coon, E.T, J.D. Moulton and S.L. Painter (2016). Managing complexity in simulations of land surface and near-surface processes. *Environmental Modelling & Software*, 78, 134-149.
- Chauhan, N. S., Miller, S., & Ardanuy, P. (2003). Spaceborne soil moisture estimation at high resolution: a microwave-optical/IR synergistic approach. *International Journal of Remote Sensing*, 24(22), 4599-4622.
- Coudert, B., Ottlé, C., & Briottet, X. (2008). Monitoring land surface processes with thermal infrared data: Calibration of SVAT parameters based on the optimisation of diurnal surface temperature cycling features. *Remote Sensing of Environment*, 112(3), 872-887.
- El-Sharkawi, A., Shouman, A., & Lasheen, S. (2013). Service Oriented Architecture for Remote Sensing Satellite Telemetry Data Implemented on Cloud Computing. *International Journal of Information Technology & Computer Science*, 5(7), 12.
- European Space Agency: Support to Science Element, a Pathfinder for Innovation in Earth Observation, ESA, available at: http://due.esrin.esa.int/stse/files/document/STSE_report_121016.pdf (last access: 10 July 2014), 2012.

353 Gillies, R. R., Kustas, W. P., & Humes, K. S. (1997). A verification of the 'triangle' method for
 354 obtaining surface soil water content and energy fluxes from remote measurements of the
 355 Normalized Difference Vegetation Index (NDVI) and surface ϵ . *International journal of*
 356 *remote sensing*, 18(15), 3145-3166.

357 Gillies, R.R., 1993. A physically-based land use classification scheme using remote solar and
 358 thermal infrared measurements suitable for describing urbanisation. PhD Thesis, University
 359 of Newcastle, UK, 121 pp.

360 Grantz, D. A., Zhang, X., & Carlson, T. (1999). Observations and model simulations link stomatal
 361 inhibition to impaired hydraulic conductance following ozone exposure in cotton. *Plant, Cell*
 362 *& Environment*, 22(10), 1201-1210.

363 Ireland, G., G.P. Petropoulos, T.N. Carlson & S. Purdy (2015): Addressing the ability of a land
 364 biosphere model to predict key biophysical vegetation characterisation parameters with
 365 Global Sensitivity Analysis Environmental Modelling & Software, 65, 94-107.

366 Jung, M., Reichstein, M., Margolis, H. A., Cescatti, A., Richardson, A. D., Arain, M. A., ... & Williams,
 367 C. (2011). Global patterns of land-atmosphere fluxes of carbon dioxide, latent heat, and
 368 sensible heat derived from eddy covariance, satellite, and meteorological observations.
 369 *Journal of Geophysical Research: Biogeosciences* (2005–2012), 116(G3).

370 Lynn, B. H., & Carlson, T. N. (1990). A stomatal resistance model illustrating plant vs. external
 371 control of transpiration. *Agricultural and Forest Meteorology*, 52(1), 5-43.

372 Mannschatz, T, T. Wolf & S. Hulsmann (2016): Nexus Tools Platform: Web-based comparison of
 373 modelling tools for analysis of water-soil-waste nexus. *Environmental Modelling & Software*,
 374 76, 137-153.

375 North, M. R., Petropoulos, G.P., Rendall, D.V., Ireland, G.I. & J.P. McCalmont (2015): Evaluating the
 376 capability of a land biosphere model in simulating land surface processes: results from
 377 different European Ecosystems. DOI: doi:10.5194/esdd-6-217-2015 *Earth Surface*
 378 *Dynamics Discussions*.

379 Petropoulos, G., Carlson, T. and Wooster, M. J. (2009a): An Overview of the Use of the SimSphere
 380 Soil vegetation Atmospheric Transfer (SVAT) Model for the Study of Land Atmosphere
 381 Interactions, *Sensors*, 9, 4286-4308.

382 Petropoulos, G., Wooster, M. J., Kennedy, K., Carlson, T.N. and Scholze, M. (2009b): A global
 383 sensitivity analysis study of the 1d SimSphere SVAT model using the GEM SA software, *Ecol.*
 384 *Model.*, 220, 2427-2440.

385 Petropoulos, G. P., Konstas, I., and Carlson, T. N (2013a): Automation of SimSphere Land Surface
 386 Model Use as a Standalone Application and Integration with EO Data for Deriving Key Land
 387 Surface Parameters, *European Geosciences Union*, 7–12 April 2013, Vienna, Austria.

388 Petropoulos, G. P., Griffiths, H., and Tarantola, S. (2013b): Sensitivity analysis of the SimSphere
 389 SVAT model in the context of EO-based operational products development, *Environ. Modell.*
 390 *Softw.*, 49, 166–179, 2013c.

391 Piles, M., Camps, A., Vall-Llossera, M., Corbella, I., Panciera, R., Rüdiger, C., ... & Walker, J. (2011).
 392 Downscaling SMOS-derived soil moisture using MODIS visible/infrared data. *Geoscience*
 393 *and Remote Sensing, IEEE Transactions on*, 49(9), 3156-3166.

394 Piles, M., G.P. Petropoulos, G. Ireland & N. Sanchez (2016): A Novel Method to Retrieve Soil
 395 Moisture at High Spatio-Temporal Resolution Based on the Synergy of SMOS and MSG
 396 SEVIRI observations. *Remote Sensing of Environment* [in press].

397 Ridler, M. E., Sandholt, I., Butts, M., Lerer, S., Mougin, E., Timouk, F, ... & Madsen, H. (2012).
398 Calibrating a soil-vegetation-atmosphere transfer model with remote sensing estimates of
399 surface temperature and soil surface moisture in a semi-arid environment. Journal of
400 Hydrology, 436, 1-12.

401 Schroth, C., & Janner, T. (2007). Web 2.0 and SOA: Converging Concepts Enabling the Internet of
402 Services. IT Professional 9, Nr. 3, pp. 36-41, IEEE Computer Society.

403 Shafranovich, Y. (October 2005). "Common Format and MIME Type for CSV Files". Network
404 Working Group (RFC 4180)

405

List of Figures:

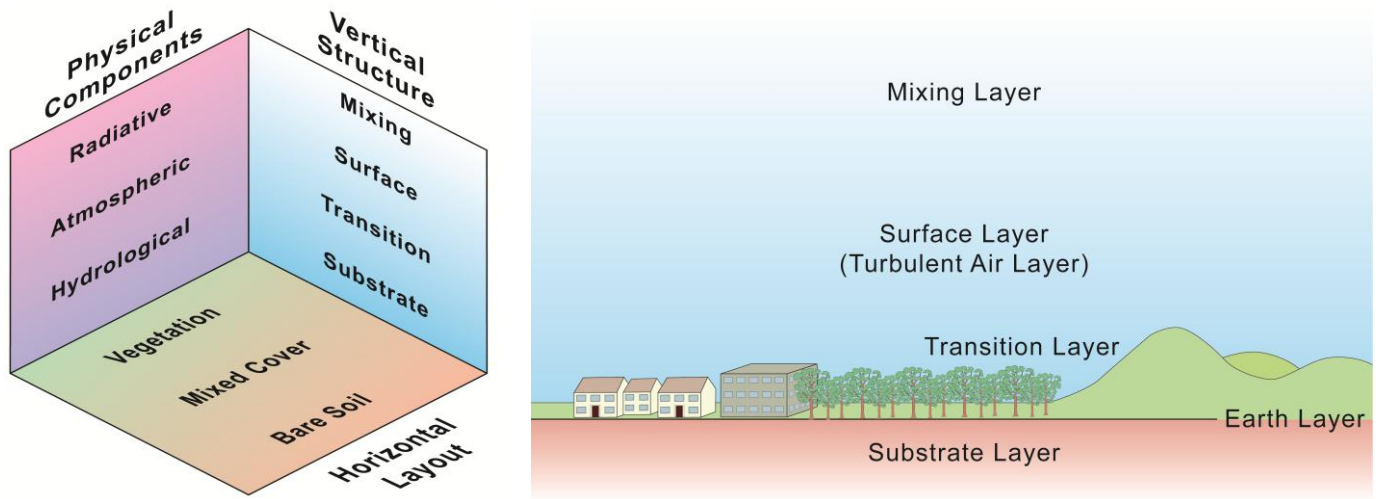


Fig 1: Basic structure of SimSphere, with the different model components summarised

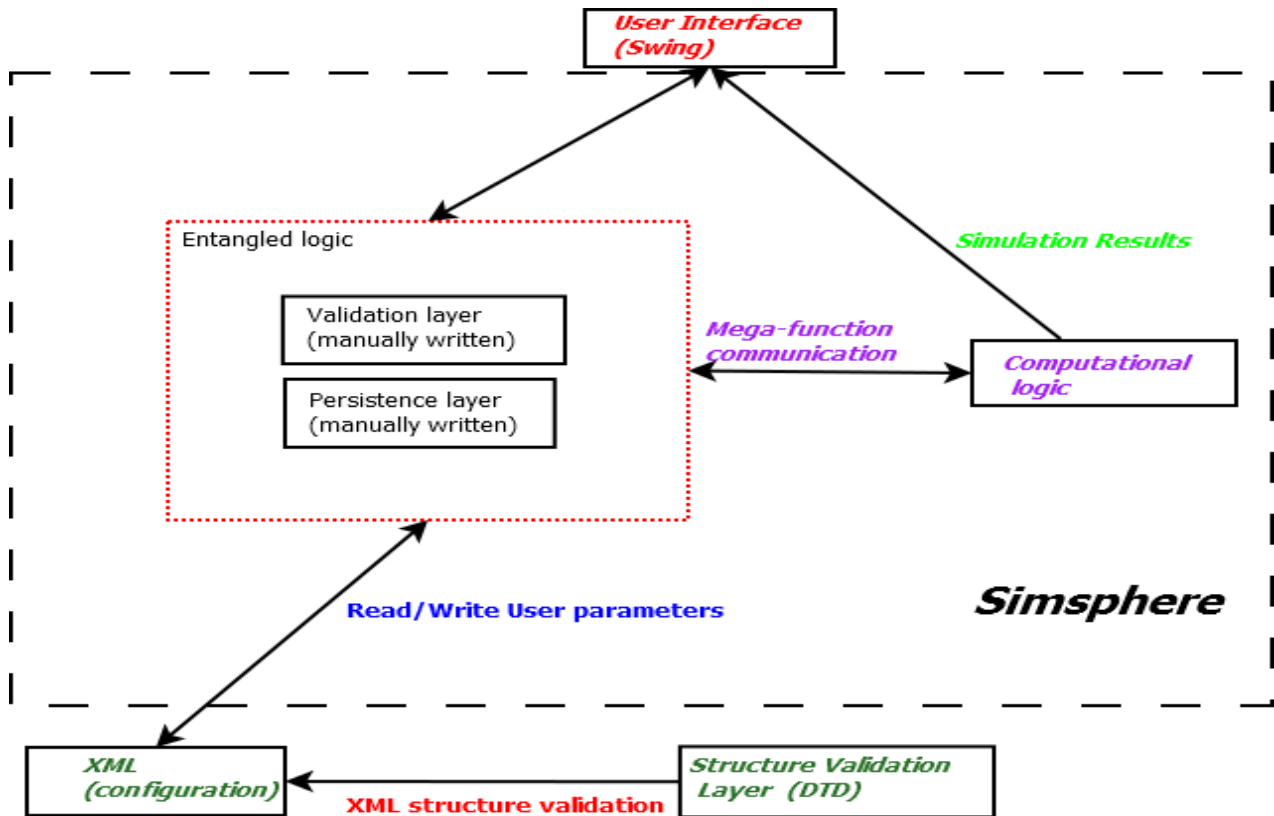


Fig. 2. Original SimSphere architecture

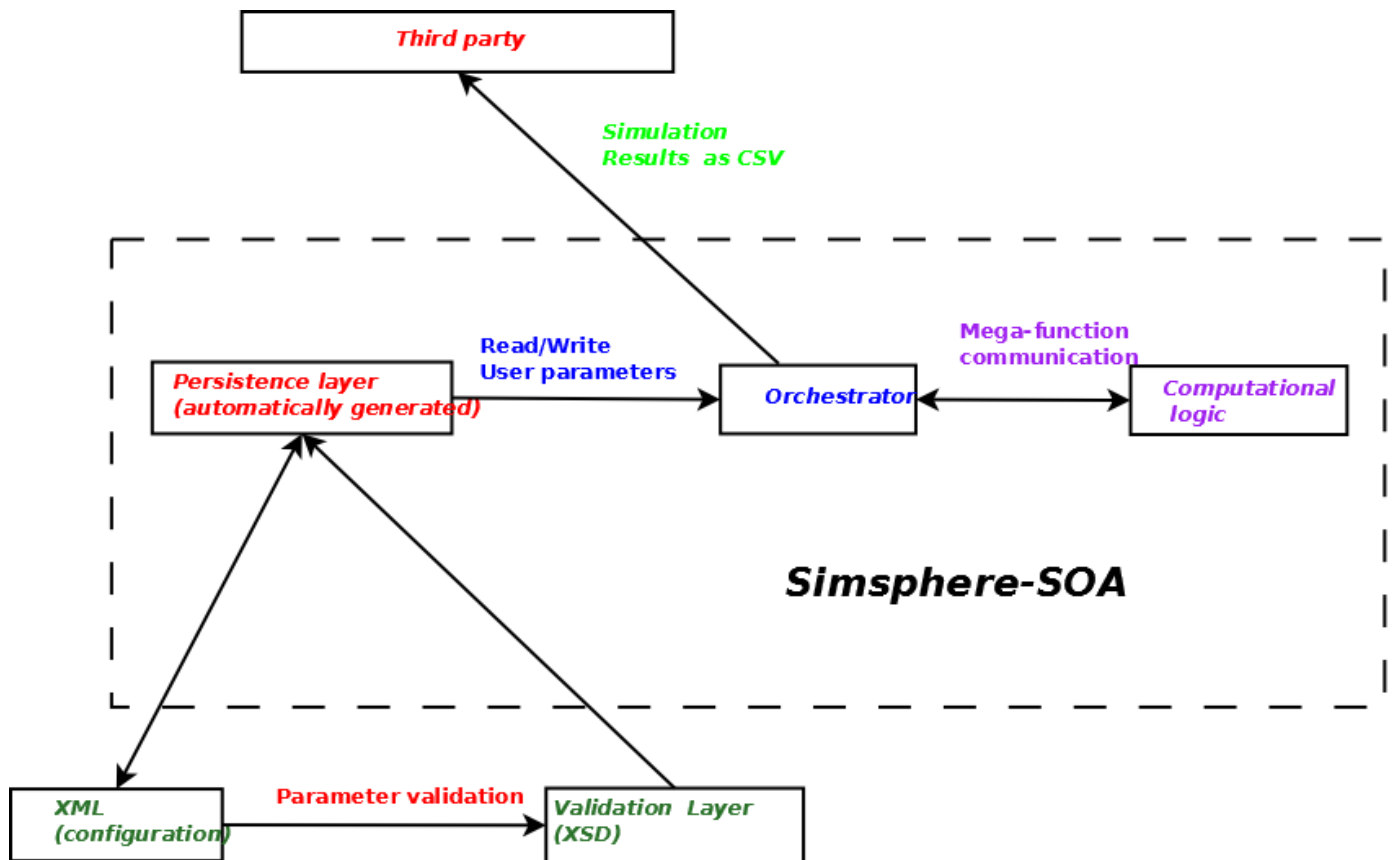


Fig. 3 The new friendly architecture of SimSphere-SOA

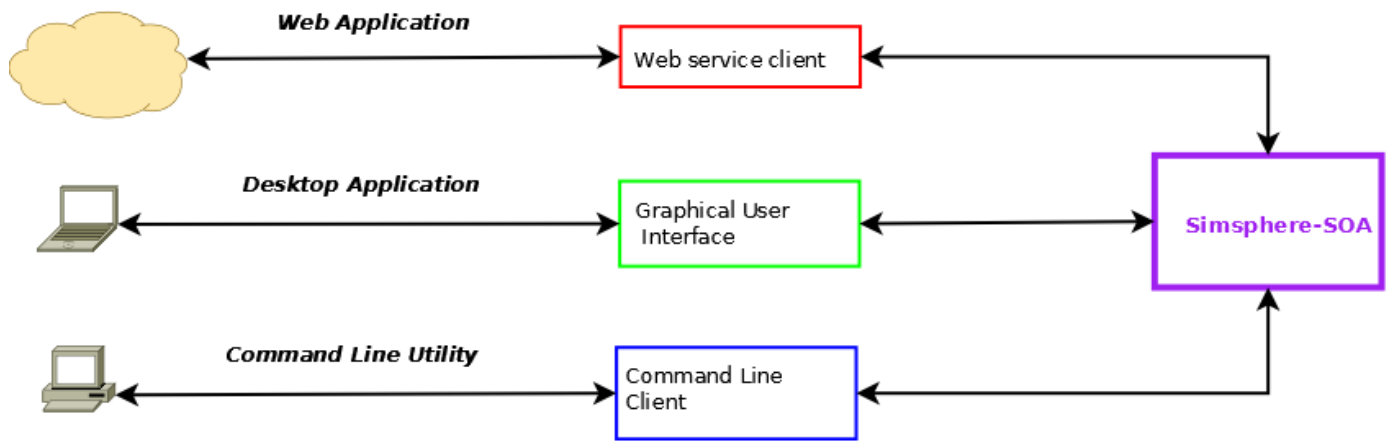


Fig. 4 Example of SimSphere-SOA applications

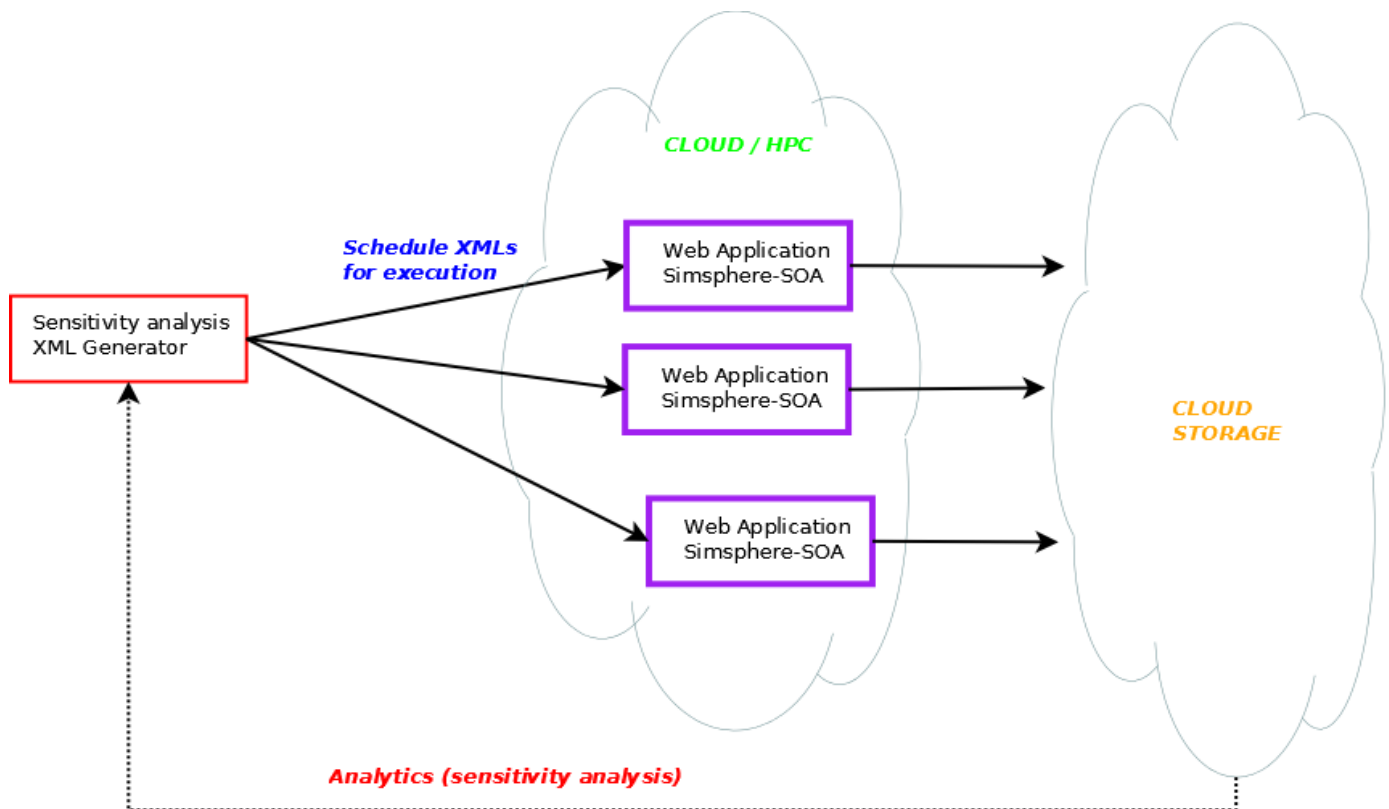


Fig. 5 SimSphere-SOA in cluster mode

```
cmd
cmd
orbit@GOPRO-PC c:\workspace
> java -jar xsd11-validator.jar -sf simsphere.xsd -if sample.xml
[Error] file:///c:/workspace/sample.xml:58:42: cvc-maxInclusive-valid: Value '20' is not facet-valid with respect to maxInclusive '1.0E1' for type 'CloudCoverType'.
[Error] file:///c:/workspace/sample.xml:58:42: cvc-complex-type-2.2: Element 'CloudCover' must have no element [children], and the value must be valid.
[Error] file:///c:/workspace/sample.xml:64:63: cvc-minInclusive-valid: Value '0' is not facet-valid with respect to minInclusive '5.0E0' for type 'MinTemperatureType'.
[Error] file:///c:/workspace/sample.xml:64:63: cvc-attribute.3: The value '0' of attribute 'MinTemperature' on element 'TemperatureRange' is not valid with respect to its type, 'MinTemperatureType'.
[Error] file:///c:/workspace/sample.xml:487:15: cvc-assertion.3.13.4.1: Assertion evaluation ('count(/simsphere:Sounding[@AltAboveStation eq 0]) gt 0') for element 'SoundingSet' with ty
'#anonymous' did not succeed.
orbit@GOPRO-PC c:\workspace
>
```

Fig. 6 Validation failure on converted xml values.

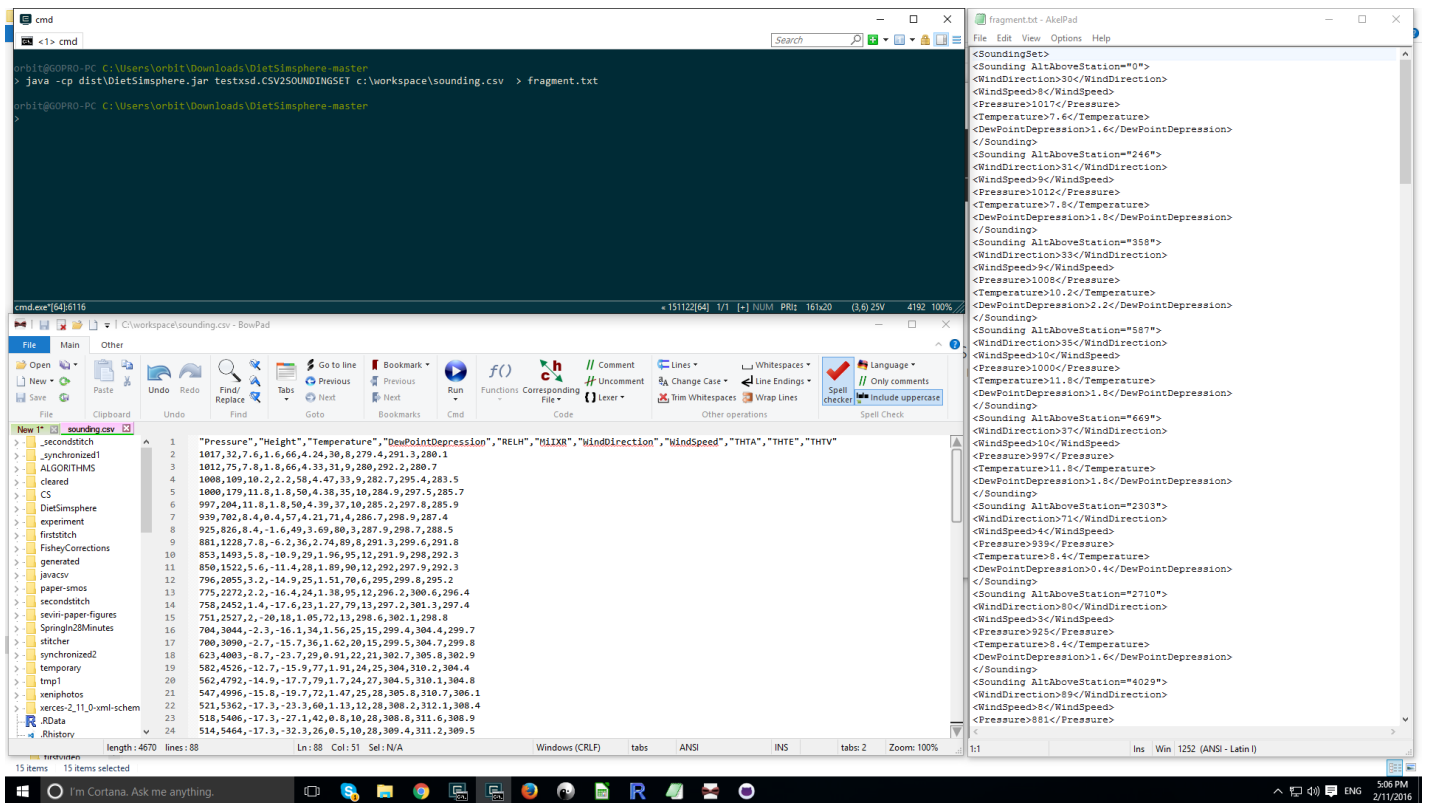


Fig. 7 XML fragment generation from imported sounding data.

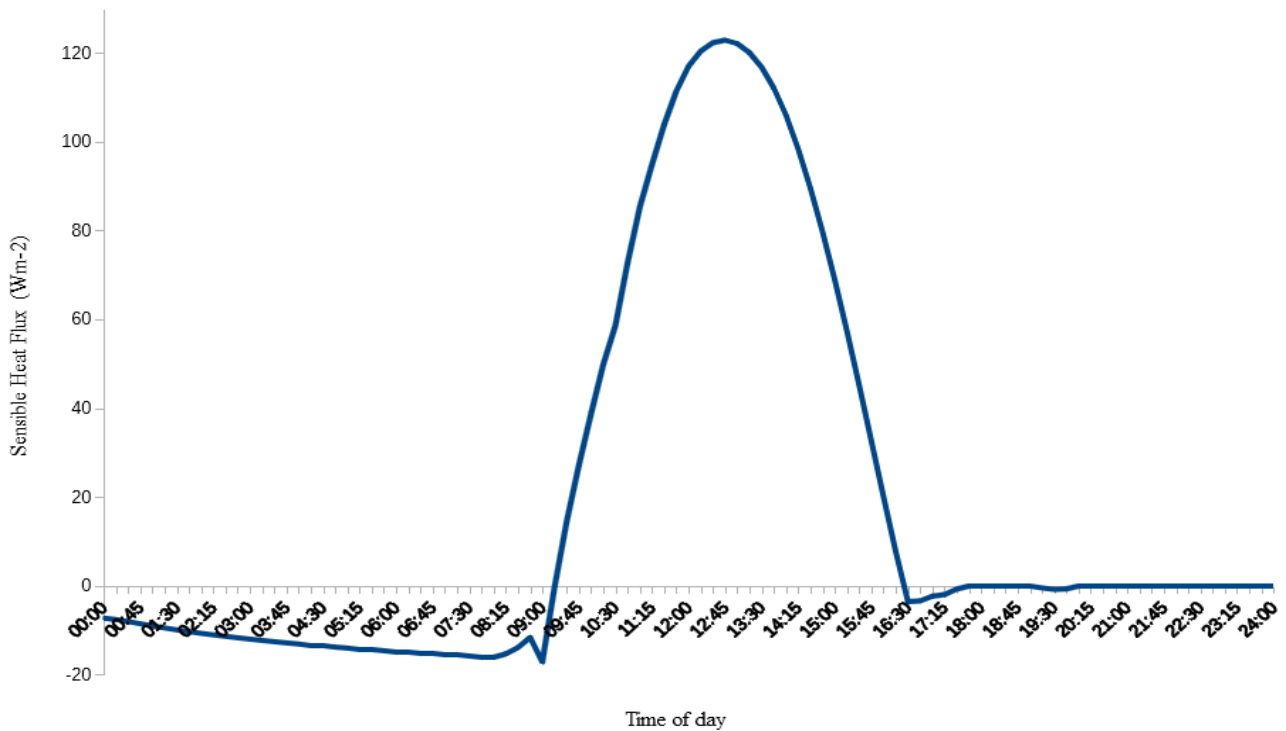


Fig. 8 Sensible Heat Flux predicted by the Simsphere-SOA

List of Tables

Table 1: Summary of the main SimSphere inputs.

NAME OF THE MODEL INPUT	PROCESS IN WHICH PARAMETER IS INVOLVED	MIN VALUE	MAX VALUE
Slope (<i>degrees</i>)	TIME & LOCATION	0	45
Aspect (<i>degrees</i>)	TIME & LOCATION	0	360
Station Height (<i>meters</i>)	TIME & LOCATION	0	4.92
Fractional Vegetation Cover (%)	VEGETATION	0	100
LAI (m^2m^{-2})	VEGETATION	0	10
Foliage emissivity (<i>unitless</i>)	VEGETATION	0.951	0.990
[Ca] (external [CO ₂] in the leaf) (<i>ppmv</i>)	VEGETATION	250	710
[Ci] (internal [CO ₂] in the leaf) (<i>ppmv</i>)	VEGETATION	110	400
[O ₃] (ozone concentration in the air) (<i>ppmv</i>)	VEGETATION	0.0	0.25
Vegetation height (<i>meters</i>)	VEGETATION	0.021	20.0
Leaf width (<i>meters</i>)	VEGETATION	0.012	1.0
Minimum Stomatal Resistance (sm^{-1})	PLANT	10	500
Cuticle Resistance (sm^{-1})	PLANT	200	2000
Critical leaf water potential (<i>bar</i>)	PLANT	-30	-5
Critical solar parameter (Wm^{-2})	PLANT	25	300
Stem resistance (sm^{-1})	PLANT	0.011	0.150
Surface Moisture Availability (<i>vol/vol</i>)	HYDROLOGICAL	0	1
Root Zone Moisture Availability (<i>vol/vol</i>)	HYDROLOGICAL	0	1
Substrate Max. Volum. Water Content (<i>vol/vol</i>)	HYDROLOGICAL	0.01	1
Substrate climatol. mean temperature ($^{\circ}C$)	SURFACE	20	30
Thermal inertia ($Wm^{-2}K^{-1}$)	SURFACE	3.5	30
Ground emissivity (<i>unitless</i>)	SURFACE	0.951	0.980
Atmospheric Precipitable water (<i>cm</i>)	METEOROLOGICAL	0.05	5
Surface roughness (<i>meters</i>)	METEOROLOGICAL	0.02	2.0
Obstacle height (<i>meters</i>)	METEOROLOGICAL	0.02	2.0
Fractional Cloud Cover (%)	METEOROLOGICAL	1	10
RKS (satur. thermal conduct. (Cosby et al., 1984))	SOIL	0	10
Cosby B (see Cosby et al., 1984)	SOIL	2.0	12.0
THM (satur.vol. water cont.) (Cosby et al., 1984)	SOIL	0.3	0.5
PSI (satur. water potential) (Cosby et al., 1984)	SOIL	1	7
Wind direction (<i>degrees</i>)	WIND SOUNDING PROFILE	0	360
Wind speed (<i>knots</i>)	WIND SOUNDING PROFILE	---	---
Altitude (<i>1000's feet</i>)	WIND SOUNDING PROFILE	---	---
Pressure (<i>mBar</i>)	MOISTURE SOUNDING PROFILE	---	---
Temperature (<i>Celsius</i>)	MOISTURE SOUNDING PROFILE	---	---
Temperature-Dewpoint Temperature (<i>Celsius</i>)	MOISTURE SOUNDING PROFILE	---	---

Table 2: Summary of the main s outputs simulated by SimSphere.

SimSphere model Outputs				
Output Name	Units		Output Name	Units
Air temperature at 1.3m	°C		Radiometric Temperature	°C
Air temperature at 50m	°C		Root Zone moisture Avail.	n/a
Air temperature at foliage	°C		Sensibel heat flux	Wm ⁻²
Bowen ratio	n/a		Short-wave flux	Wm ⁻²
[CO ₂] on canopy	ppmv		Specific humidity at 1.3m	gKg ⁻¹
[CO ₂] flux	micromolesm ² s ⁻¹		Specific humidity at 50m	gKg ⁻¹
Epidermal water potential	Bars		Specific humidity at foliage	gKg ⁻¹
Global O ₃ flux	Ugm ⁻² s ⁻¹		Stomatal resistance	sm ⁻¹
Ground flux	Wm ⁻²		Surface moisture availability	n/a
Ground water potential	bars		Vapor pressure deficit	Mbar
Latent Heat flux	Wm ⁻²		Water Use Efficiency	n/a
Leaf water potential	bars		Wind at 10m	Kts
Net Radiation	Wm ⁻²		Wind at 50m	Kts
[O ₃] canopy	ppmv		Wind in foliage	Kts
[O ₃] flux plant	Ugm ⁻² s ⁻¹			

Table 3. Web service endpoints of SimSphere-SOA

Endpoint	Description	Method
http://localhost:8080/timebased	Time based	POST
http://localhost:8080/convolution	Convolution simulation	POST

Table 4: Two examples XSD 1.1 assertions used

Description	Assertion
Altitude above station must start at 0	<code><xsd:assert test="count(/simsphere:Sounding[@AltAboveStation eq 0]) gt 0"/></code>
Minimum temperature must be below maximum temperature.	<code><xsd:assert test="@MinTemperature le @MaxTemperature"/></code>

Table 5: The longitude definition as used by SimSphere-SOA

<code><xsd:element name="Longitude"></code>
<code> <xsd:annotation></code>
<code> <xsd:documentation></code>
<code> The longitude in degrees.</code>
<code> </xsd:documentation></code>
<code> </xsd:annotation></code>
<code> <xsd:simpleType></code>
<code> <xsd:restriction base="xsd:float"></code>
<code> <xsd:minInclusive value="-180"/></code>
<code> <xsd:maxInclusive value="180"/></code>
<code> </xsd:restriction></code>
<code> </xsd:simpleType></code>
<code></xsd:element></code>

Table 6. Comparison of old and new approaches in providing the longitude parameter in XML input

Approach	Code
OLD	<pre> <ParamLabel Format="##0.##" Label="Longitude (deg)" ParmElem="Longitude"> </ParamLabel> <Longitude Value="96.55"> <BoundedRange MaxType="closed" Maximum="180" MinType="closed" Minimum="-180" RangeID="ID102"> </BoundedRange> </Longitude> </pre>
NEW	<pre> <Longitude>96.55</Longitude> </pre>

Table 7: Analysis using CLOC of old and new serialization and validation codebases

Approach	Files	Blanks	Comments	Lines of Code	File Size
OLD (Java only serialization)	38	1152	2069	4393 (manual)	
NEW (Java only)	0	N/A	N/A	0 (manual)	
OLD (DTD only)	1	N/A	N/A	311	
NEW (XSD only)	1	N/A	N/A	1145	
OLD XML Input					106KB
NEW XML Input					26KB